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NEA TDBIV PROJECT: PREPARATION OF A STATE-OF-THE-ART REPORT ON THERMODYNAMIC DATA FOR CEMENTS

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The program of work of the fourth phase of the OECD NEA Thermochemical Database Project (TDB-IV) contemplates a line of activity on the preparation of a state of the art report on cements. The present work aims at presenting the project, its aims and its limits.

In the context of nuclear waste disposal, concrete is used both as a confinement and a building material. The safety of the repository has to be assessed over long period of times. Numerical simulations remain an important tool for such an assessment. For that purpose, the stability and more precisely, the solubilities of the mineral that compose the different containment barriers have to be defined with reliability, by taking into account the experimental data published on this topic. The present project aims to provide a consistent and reliable set of thermodynamic parameters especially for the minerals that form in cementitious materials. It consists in a review of the literature in order to establish what chemical thermodynamic data, models and numerical implementation tools exist for the thermodynamic treatment of cement systems. The chemical system considered contains Na_2O-K_2O-CaO-SiO_2-Al_2O_3-MgO-Fe_2O_3-CO_2-SO_3-Cl-H_2O and includes nanocrystalline and crystalline phases. In addition, since high-level long lived radwaste and some of the intermediate level wastes are exothermic (e.g. compacted hulls and endspecies), temperature exposure of the concrete backfill and packages must be considered. To describe the solubility at a range of temperatures, a complete set of thermodynamic parameters, including entropies and heat capacities functions, is needed.

The review itself covers the fields of:

- C-S-H minerals. This includes noncrystalline and crystalline phases, Al, Fe and Mg substitutions, the influence of relative humidity
- AFm, AFt, Hydrogarnet solid solutions
- Additional phases, hydroxides, zeolites

The work concerns basically the thermodynamics properties of minerals. Surface reactions or the influence of kinetics will not be treated. .